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From Random Fields to Classical or Generalized Continuum Models

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The main motivation for developing a stochastic multiscale mechanics stems from the recognition that the material microstructure/composition is, in general, random and involves two or more scales. These issues are discussed here from the standpoint of (i) random fields of material properties, and (ii) the choice of classical versus non-classical continua. The topic (i) hinges on a theoretical approach based on a Hill-Mandel condition which, for any body B_δ having no holes or rigid inclusions, guarantees the equivalence of energetically and mechanically defined effective responses

$$\overline{\int \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}} = \int \bar{\boldsymbol{\sigma}} : d\bar{\boldsymbol{\varepsilon}} \Leftrightarrow \int_{\partial B_\delta} (\mathbf{t} - \bar{\boldsymbol{\sigma}} \cdot \mathbf{n}) \cdot (d\mathbf{u} - d\bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x}) dS = 0, \quad (1)$$

Here ∂B_δ is the boundary of B_δ and δ is the mesoscale [1]. This equation suggests three special types of uniform boundary conditions (BCs):

$$(i) \text{ uniform displacement BC: } d\mathbf{u} = d\bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x} \quad (2)$$

$$(ii) \text{ uniform traction BC: } \mathbf{t} = \bar{\boldsymbol{\sigma}} \cdot \mathbf{n} \quad (3)$$

$$(iii) \text{ uniform mixed-orthogonal BC: } (\mathbf{t} - \bar{\boldsymbol{\sigma}} \cdot \mathbf{n}) \cdot (d\mathbf{u} - d\bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x}) = 0 \quad (4)$$

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By increasing the mesoscale δ (effectively, the number of grains in B_δ) and by setting up stochastic boundary value problems with the above boundary conditions and upon ensemble averaging, one obtains bounds on the constitutive response of the aggregate. Now, the condition (2) results in a mesoscale (i.e. δ -dependent) stiffness tensor \mathbf{C}_δ^d , (3) in a mesoscale compliance tensor \mathbf{S}_δ^t , while (4) yields a mesoscale conductivity or resistivity tensor (depending on a specific interpretation). The superscripts d and t denote quantities obtained under essential and natural BCs, respectively.

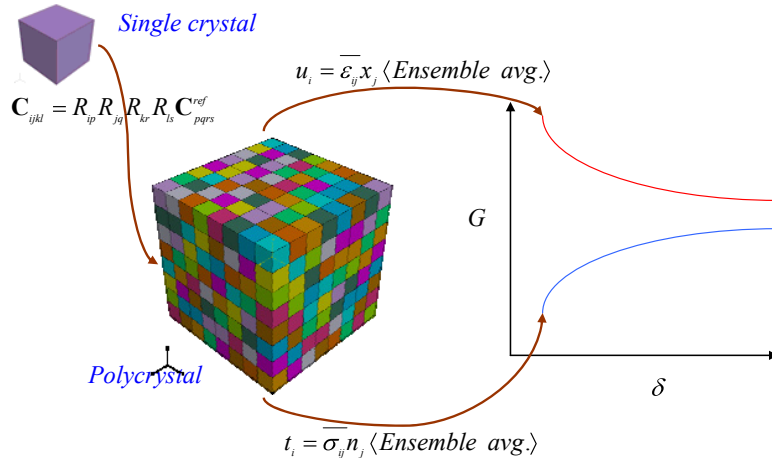


Figure 1. Methodology to obtain scale-dependent bounds for elastic polycrystals [2,3].

The application of (1) to bodies B_δ at various mesoscales allows a determination of scaling laws and mesoscale random fields with continuous realizations from the microscale material properties typically described by random fields with discontinuous realizations. The latter appear in image analyses of just about any microstructure (composite, polycrystalline, granular,...). This ensures physically consistent models of random fields for a wide range of elastic or inelastic, linear or nonlinear, and possibly multifield settings [1,2,3]. The mesoscale random fields – in the vein of ideas outlined in [4] – then enter stochastic field equations and finite element, finite difference, or even boundary element methods. We next discuss one- and two-point statistics, the (an)isotropy of realizations versus (an)isotropy of correlation functions, as well as their unavoidable scale-dependence, non-uniqueness, and correspondence with specific variational principles of solid mechanics [5,6].

In the case when the mesoscale information of higher quality than that offered by the classical continuum is desired, the scale-dependent homogenization involves mesoscale random fields of, say, micropolar type. Another scenario arises when impact phenomena are involved: kinetic energies have to be accounted for when upscaling from the microstructural

level [7]. In both cases, an approach generalizing the Hill-Mandel condition provides a link between the microscale and the macroscale.

In some deterministic mechanics problems there is a definite advantage to working with non-local continuum formulations. Two models are possible: a non-local statement of the constitutive law along with a well-known statement of other governing equations (Eringen's approach [8]) or a peridynamic model (Kunin-Rogula-Silling's approach [9,10,11]) where the equation of motion is written directly as a volume integral grasping the spatial discontinuities without ambiguous interpretations of spatial derivatives. The key question here is: How can such models be generalized to stochastic settings consistent with the principles of mechanics?

More generally, the presence of dissipative phenomena in mechanics of materials necessitates a formulation of continuum theories consistent with thermodynamics, leading to stochastic thermomechanics. Given the four (deterministic) continuum thermomechanics theories: thermodynamics of irreversible processes (TIP), thermodynamics with internal variables (TIV); rational thermodynamics (RT); extended (rational) thermodynamics (ET), we examine how they can be generalized so as to account for upscaling from random microstructure to mesoscale random fields, e.g. [12]. In all the cases above, the key role is played by a statistical (rather than a representative) volume element, which leads to an optimal finite element size.

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